

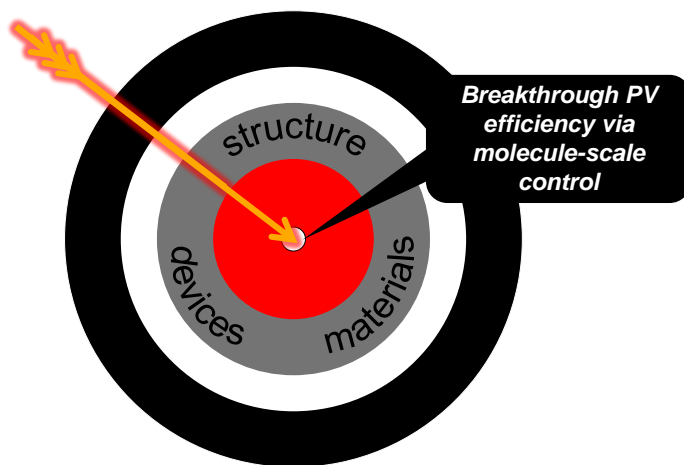
Re-Defining Photovoltaic Efficiency Through Molecule Scale Control (RPEMSC)

EFRC Director(s): James Yardley, Tony Heinz, Louis Brus

Lead Institution: Columbia University

Mission Statement: The Columbia EFRC will create critical enabling technology which will redefine thin film photovoltaic efficiency through development of fundamental understanding based upon molecule-scale control of the key steps in the photovoltaic process for organic and hybrid materials.

The primary approach of the EFRC is to develop new fundamental understanding that will enable the development of revolutionary highly-efficient inexpensive photovoltaic solar cells. The EFRC will focus its expertise in chemical synthesis, fabrication, manipulation, and characterization of nanoscale materials and materials theory in order to: (1) systematically develop the fundamental understanding of the primary photovoltaic processes in organic and hybrid materials needed to advance the efficiency of inexpensive solar cells toward the well-known Shockley-Queisser efficiency limit; and (2) develop and quantitatively investigate new nanostructured materials with potential for extracting multiple electrical charges from a single absorption event thus establishing a scientific basis for moving the efficiency of these solar cell devices well beyond the Shockley-Queisser efficiency limit. The new understanding and novel nanomaterials developed by this research team will play a key role in enabling the development highly-efficient solar energy technologies. The research program of the EFRC centers around three multi-site, multi-disciplinary, and interlocking research thrusts. Each thrust represents an integrated effort incorporating theory, materials, and measurement.



Thrust 1 is dedicated to “Charge Generation: Excitation, Separation, and Extraction of Charge Carriers in Tailored Nanostructures.” In this thrust we are developing a set of new, chemically well-characterized nanoscale materials. These include new quantum dots including asymmetric quantum dots and a set of novel chemical compounds that we call “molecular clusters.” We are quantifying the dynamics and effectiveness of fundamental photophysical processes in these materials, using modern tools of Nanoscale science including ultrafast and single molecule spectroscopies. We are studying the structure of interfaces of new and novel thin film semiconductor materials with other semiconductors as well as with metals. Based on these interfaces, we are correlating the charge transport characteristics at interfaces with the observed structure. We are also building a theoretical framework to model kinetic processes of charge transport, with input from atomic scale calculation of local bonding, structure, and electronic states. We are measuring the effectiveness of charge transport across interfaces using a variety of techniques including photoemission.

Thrust 2 examines aspects of “Charge Collection: Transport at the Nanoscale and Beyond.” In this thrust we are building new materials suitable for studying the fundamental physics in bulk heterojunction solar cell devices including new chemically-tailored semiconductor materials and ordered interfaces. We are developing theoretical models for exciton dissociation, diffusion, and separation in these structures. We

support these models with nanofabricated devices using both top-down and bottom-up approaches. We directly measure charge transport in these systems. We are examining the efficacy of new carbon-based conductor materials including graphene for use as transparent conducting materials for efficient extraction of charge from thin film photovoltaic devices. These activities merge to allow us to fabricate new devices and device structures for direct determination of photovoltaic characteristics in working devices. One example shown in Figure 1 is a novel “transparent” solar cell device using transparent graphene electrodes for both cathode and anode.

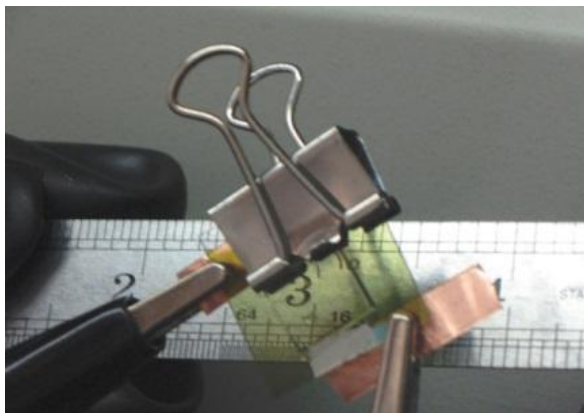


Figure 1. Transparent photovoltaic cell using graphene for both anode and cathode.

Thrust 3 explores “Carrier Multiplication: Beyond the Shockley-Queisser Limit.” Our program is first working to identify clear experimental signatures for multi-exciton generation (MEG) and related singlet fission processes for producing multiple charge carriers. We are developing structures and materials for optimal carrier multiplication schemes including MEG. This involves systematic exploration of MEG and related phenomena in quantum dot and carbon-based systems such as graphene nanoribbons or carbon nanotubes using direct charge carrier detection as well as a variety of spectroscopic techniques. In addition we are exploring theoretically generic concepts for carrier multiplication processes. This will allow us to establish a quantitative and predictive theory for MEG and related carrier multiplication concepts. This theory will guide our experimental program in terms of systems under study and materials used in these systems.

Center for Re-Defining Photovoltaic Efficiency Through Molecule Scale Control	
Columbia University	James Yardley (Managing Director), Louis Brus (Scientific Director), Tony Heinz (Scientific Director), Simon Billinge, Luis Campos, George Flynn, Irving Herman, James Hone, Philip Kim, Ioannis Kymissis, Colin Nuckolls, Richard Osgood, Jonathan Owen, David Reichman, Kenneth Shepard, Michael Steigerwald, Latha Venkataraman, Chee Wei Wong
Purdue University	Ashraf Alam
University of Texas	Xiaoyang Zhu
Brookhaven National Laboratories	Charles Black, Mark Hybertsen

Contact: James T. Yardley
Professor, Electrical Engineering
Email: jy307@columbia.edu
Telephone: 212-854-3839
EFRC Website: www.cise.columbia.edu/efrc/